Toluene
108-88-3 | DTXSID7021360

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.00e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.32e-01

Confidence level: 7.31e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
1,3,5-Cycloheptatriene	Propane, 2-iodo-	Diethyl disulphide
Measured: 6.73e-03	**Measured:** 8.24e-03	**Measured:** 2.45e-03
Predicted: 4.23e-03	**Predicted:** 8.51e-03	**Predicted:** 3.63e-03